

# INFORMATION THEORY AND STATISTICAL MECHANICS REVISITED

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**ABSTRACT.** We derive Bose-Einstein statistics and Fermi-Dirac statistics by Principle of Maximum Entropy applied to two families of entropy functions different from the Boltzmann-Gibbs-Shannon entropy. These entropy functions are identified with special cases of modified Naudts'  $\phi$ -entropy.

In a pioneering work sixty years ago, Jaynes [4] initiated the study of statistical physics by information theory. He expounded the Principle of Maximum Entropy and applied it to Boltzmann-Gibbs-Shannon entropy to derive Boltzmann-Gibbs statistics. Many different entropy functionals have been introduced, studied and used in many areas where statistics have been applied. But in physics, only the Boltzmann-Gibbs-Shannon entropy has been considered as “physical”. Tsallis [7] has proposed the  $q$ -entropy as another kind of physical entropy functional. Naudts [6] introduced  $\phi$ -exponentials,  $\phi$ -logarithms and  $\phi$ -entropy as a further generalization related to the  $q$ -entropy. On [6, p. 94] he wrote: “One of the conclusions is that the  $q$ -deformed exponential family occurs in a natural way within the context of classical mechanics. The more abstract generalisations discussed in the final chapters may seem less important from a physics point of view. But they have been helpful in elucidating the structure of the theory of generalised exponential families.” We will show that such generalizations are indeed of physical importance, in particular, in understanding the Bose-Einstein statistics and the Fermi-Dirac statistics by Principle of Maximum Entropy.

We will first consider the subjective statistical physics of free bosons and free fermions. More precisely, we will derive Bose-Einstein statistics and Fermi-Dirac statistics from the Principle of Maximum Entropy, not for the Boltzmann-Gibbs-Shannon entropy as Jaynes did for the Boltzmann-Gibbs statistics, but instead for two different entropy functions. We quote here Tsallis [7, p. 4]: “Indeed, the physically important entropy - a crucial concept - is *not* thought as being an universal functional that is given once for ever, but it rather is a delicate and powerful concept to be carefully constructed for classes of

systems.” We will actually consider two different families interpolating the Bose-Einstein and Fermi-Dirac statistics. They give us two families of entropy functions.

Next we will present a unified understanding of the Boltzmann-Gibbs weight function, the Bose-Einstein weight function and the Fermi-Dirac weight function from the point of view of natural parameters of exponential families.

Finally, the three entropy functions and the three weight functions are unified in terms of special cases of the generalized logarithmic functions and generalized exponential functions developed by Naudts, respectively. Some modifications are introduced for this purpose.

We also briefly treat the case of fractional exclusion statistics [3, 8]. In a subsequent work we will treat the case of general statistics interpolating the Bose-Einstein and Fermi-Dirac statistics.

# 1. UNIFIED DERIVATION OF BOLTZMANN-GIBBS STATISTICS, BOSE-EINSTEIN STATISTICS AND FERMI-DIRAC STATISTICS FROM PRINCIPLE OF MAXIMUM ENTROPY

In this section we will introduce the statistical manifolds that describe a single particle, in finitely many states. Then we will use suitable entropy functions on these manifolds and the Principle of Maximum Entropy to give a unified derivation of three important physical statistics that describe noninteracting particles.

**1.1. The statistical manifold.** Suppose that one is performing a test with one observable  $\mathcal{E}$  with finitely many outcomes  $\{E_1, \dots, E_n\}$ ,  $E_1 < \dots < E_n$ . Suppose that each outcome has a positive probability  $p_i$  of appearance:

$$(1) \quad p(\mathcal{E} = E_i) = p_i, \quad p_i > 0, \quad i = 1, \dots, n;$$

these probabilities are required to summed up to one:

$$(2) \quad p_1 + \dots + p_n = 1.$$

Such a distribution is called a *categorical distributions* in statistics. Putting all the possible probability distributions together, one gets an open  $(n - 1)$ -simplex:

$$(3) \quad P_n = \{(p_1, \dots, p_n) \in \mathbb{R}^n \mid p_1 + \dots + p_n = 1, \quad p_i > 0, \quad i = 1, \dots, n\}.$$

It is an open  $(n - 1)$ -dimensional manifold. We will take  $p_1, \dots, p_{n-1}$  as coordinates on  $P_n$ , and express  $p_n$  as a function in these coordinates:

$$(4) \quad p_n = 1 - p_1 - \dots - p_{n-1}.$$

As in Jaynes [4] one actually works with some submanifolds of  $P_n$ , denoted by  $P_n(E_1, \dots, E_n; E)$  and defined by the following constraint:

$$(5) \quad p_1 E_1 + \dots + p_n E_n = E,$$

where  $E$  satisfies

$$(6) \quad E_1 = \min\{E_1, \dots, E_n\} \leq E \leq \max\{E_1, \dots, E_n\} = E_n.$$

**1.2. The entropy functions.** Recall the Boltzmann-Gibbs-Shannon entropy function is defined by:

$$(7) \quad H_{BGS} = - \sum_{i=1}^n p_i \log p_i.$$

We now introduce the following two entropy functions:

$$(8) \quad H_{BE} = \sum_{i=1}^n ((p_i + 1) \ln(p_i + 1) - p_i \ln p_i),$$

$$(9) \quad H_{FD} = \sum_{i=1}^n ((p_i - 1) \ln(1 - p_i) - p_i \ln p_i).$$

The motivation for the introduction of these functions will be elaborated elsewhere. Here let us just say  $H_{BE}$  can be thought of as a discrete version of [9, (14)].

We also introduce a family of entropy functions:

$$(10) \quad H_\epsilon = \sum_{i=1}^n \left( \frac{1}{\epsilon} (1 + \epsilon p_i) \ln(1 + \epsilon p_i) - p_i \ln p_i \right).$$

Then we have

$$(11) \quad H_1 = H_{BE}, \quad H_0 = H_{BGS} + 1, \quad H_{-1} = H_{FD}.$$

**1.3. Principle of Maximum Entropy.** We now show that the application of Principle of Maximum Entropy to the three entropy functions in last subsection on the statistical manifold  $P_n(E_1, \dots, E_n)$  gives us a unified derivation of the Boltzmann-Gibbs statistics, Bose-Einstein statistics, Fermi-Dirac statistics, and more generally, Acharya-Swamy statistics [1].

**Theorem 1.1.** *On  $P_n(E_1, \dots, E_n; E)$ , the entropy function  $H_\epsilon$  achieves its maximum at the points:*

$$(12) \quad p_i(\epsilon) = \frac{1}{e^{a+bE_i} - \epsilon}, \quad i = 1, \dots, n$$

for some constants  $a$  and  $b$ .

*Proof.* By the method of Lagrange multiplier, consider the function

$$\begin{aligned} F_\epsilon &= \sum_{i=1}^n \left( \frac{1}{\epsilon} (1 + \epsilon p_i) \ln(1 + \epsilon p_i) - p_i \ln p_i \right) \\ &+ a \left( 1 - \sum_{i=1}^n p_i \right) + b \left( E - \sum_{i=1}^n p_i E_i \right). \end{aligned}$$

One easily gets:

$$(13) \quad \frac{\partial F_\epsilon}{\partial p_i} = \ln \frac{1 + \epsilon p_i}{p_i} - a - b E_i, \quad i = 1, \dots, n,$$

so the critical point where  $\frac{\partial F_\epsilon}{\partial p_i} = 0$  for all  $i = 1, \dots, n$  is given by

$$(14) \quad p_i(\epsilon) = \frac{1}{e^{a+bE_i} - \epsilon}.$$

The entries of Hessian matrix of  $F_\epsilon$  are given by:

$$(15) \quad \frac{\partial^2 F_\epsilon}{\partial p_i \partial p_j} = -\delta_{ij} \frac{1}{p_i(1 + \epsilon p_i)},$$

the Hessian is clearly negatively definite.  $\square$

## 2. WEIGHT FUNCTIONS AS INVERSE FUNCTIONS OF NATURAL PARAMETERS OF EXPONENTIAL FAMILIES

In this section we understand the weight functions:

$$(16) \quad p_\epsilon(E) = \frac{1}{e^{a+bE} - \epsilon}$$

as inverse functions of natural parameters of exponential families.

**2.1. Exponential family.** In statistics, an *exponential family* of probability densities is an  $n$ -dimensional model  $S = \{p_\theta\}$  of the form

$$(17) \quad p(x; \theta) = \exp \left[ C(x) + \sum_{i=1}^n \theta^i T_i(x) - \psi(\theta) \right].$$

The parameters  $\{\theta^i\}$  are called the *natural parameters*, and the function  $\psi(\theta)$  is determined by the normalization condition

$$(18) \quad \int p(x; \theta) dx = 1,$$

and so it is given by:

$$(19) \quad \psi(\theta) = \log \int \exp \left[ C(x) + \sum_{i=1}^n \theta^i T_i(x) \right].$$

Recall when Gibbs [2] introduced the canonical ensemble in 1901 he postulated a distribution of the form

$$(20) \quad p(E) = \exp(G - \beta E)$$

where  $G$  is a normalization constant and where the control parameter  $\beta = \frac{1}{kT}$  is the inverse temperature. This is an example of exponential family.

**2.2. Boltzmann-Gibbs weight functions as inverse natural parameters for the categorical distribution.** The categorical distribution is an example of the exponential families. First one can rewrite it in the following form:

$$(21) \quad p = p_1^{[\mathcal{E}=E_1]} \cdots p_n^{[\mathcal{E}=E_n]},$$

where  $[\mathcal{E} = E_i]$  is the indicating function that equals to one when the energy level is  $E_i$ , zero otherwise. Note

$$(22) \quad \log p = \sum_{i=1}^n [\mathcal{E} = E_i] \ln p_i = \sum_{i=1}^n [\mathcal{E} = E_i] \cdot \ln p_i.$$

So by comparing with (17), one can take  $T_i = [\mathcal{E} = E_i]$ , and the natural parameters can be taken to be:

$$(23) \quad \eta_i = \ln p_i,$$

and so

$$(24) \quad p_i = e^{\eta_i}.$$

This gives us the Boltzmann-Gibbs weight function when we take  $\eta_i = -(a + bE_i)$ .

**2.3. Fermi-Dirac weight function as inverse natural parameter for the Bernoulli distribution.** The Fermi-Dirac weight function can be interpreted as the inverse function of natural parameter of the Bernoulli distribution. By Pauli's Exclusion Principle, the outcome for observing a free fermion at a fixed state is like the toss of coins, it can be only be 0 or 1 particle at this state. Suppose the probability is given by:

$$(25) \quad p(X = 1) = p, \quad p(X = 0) = 1 - p.$$

The distribution can be written as

$$(26) \quad P(X = x) = p^x (1 - p)^{1-x}.$$

This is called the *Bernoulli distribution* in statistics. This is also an example of exponential families:

$$(27) \quad \log P = x \ln \frac{p}{1-p} + \ln(1-p).$$

The natural parameter is given by:

$$(28) \quad \eta = \ln \frac{p}{1-p},$$

and so the inverse function is given by:

$$(29) \quad p = \frac{1}{e^{-\eta} + 1}.$$

This is the Fermi-Dirac weight function when we take  $\eta = -(a + bE)$ .

**2.4. The Acharya-Swamy weight function for  $\epsilon < 0$  as inverse natural parameter for the Bernoulli distribution.** In the case of  $\epsilon < 0$ , consider the probability distribution given by:

$$(30) \quad P(X = x) = \left( \frac{p}{1 + (1 + \epsilon)p} \right)^x \cdot \left( \frac{1 + \epsilon p}{1 + (1 + \epsilon)p} \right)^{1-x},$$

supported on the set  $\{0, 1\}$ . This is a curved Bernoulli distribution. This is also an example of exponential families:

$$(31) \quad \log P = x \ln \frac{p}{1 + \epsilon p} + \ln \left( \frac{1 + \epsilon p}{1 + (1 + \epsilon)p} \right).$$

The natural parameter is given by:

$$(32) \quad \eta = \ln \frac{p}{1 + \epsilon p},$$

and so the inverse function is given by:

$$(33) \quad p = \frac{1}{e^{-\eta} - \epsilon}.$$

This gives the Acharya-Swamy weight function for  $\epsilon < 0$  when we take  $\eta = -(a + bE)$ .

**2.5. The Bose-Einstein weight function as inverse natural parameter of the geometric distribution.** Similarly, the Bose-Einstein weight function can be interpreted as the inverse function of natural parameter of the geometric distribution. The number of a free boson at a fixed state can be any nonnegative integer  $n \geq 0$ . Suppose the probability is given by:

$$(34) \quad P(X = n) = \frac{p^n}{(p + 1)^{n+1}}, n = 0, 1, 2, \dots$$

This is called the *geometric distribution* in statistics. Since

$$(35) \quad \ln P(X = x) = \ln \frac{p^x}{(p+1)^{x+1}} = x \ln \frac{p}{p+1} + \ln \frac{1}{p+1},$$

one sees that it is an exponential family with natural parameter:

$$(36) \quad \eta = \ln \frac{p}{p+1},$$

with inverse function:

$$(37) \quad p = \frac{1}{e^{-\eta} - 1}.$$

This is the Bose-Einstein weight function when we take  $\eta = -(a + bE)$ .

**2.6. The Acharya-Swamy weight function for  $\epsilon > 0$  as inverse natural parameter for the geometric distribution.** Consider the probability distribution given by:

$$(38) \quad P(X = n) = \frac{(p/(1 + (\epsilon - 1)p))^n}{((1 + \epsilon p)/(1 + (\epsilon - 1)p))^{n+1}}, n = 0, 1, 2, \dots$$

This is a curved geometric distribution. Since

$$(39) \quad \ln P(X = x) = x \ln \frac{p}{1 + \epsilon p} + \ln \frac{1 + (\epsilon - 1)p}{1 + \epsilon p},$$

one sees that it is an exponential family with natural parameter:

$$(40) \quad \eta = \ln \frac{p}{1 + \epsilon p},$$

with inverse function:

$$(41) \quad p = \frac{1}{e^{-\eta} - \epsilon}.$$

This is the Acharya-Swamy weight function for  $\epsilon > 0$  when we take  $\eta = -(a + bE)$ .

### 3. BOSE-EINSTEIN STATISTICS AND FERMI-DIRAC STATISTICS AS GENERALIZED STATISTICAL PHYSICS

The discussions of exponential families in last section serve as a psychological vehicle that takes us to the notion of generalized exponential families developed by Naudts [6], which generalizes the  $q$ -exponential families of Tsallis [7]. We first recall the  $\phi$ -logarithm function, the  $\phi$ -exponential function and the  $\phi$ -entropy function, then we use their suitable modifications to study  $H_\epsilon$  and  $p_\epsilon$ .

**3.1. The  $\phi$ -logarithm.** Fix a strictly positive non-decreasing function  $\phi(u)$ , defined on the positive numbers  $(0, +\infty)$ . It can be used to define a deformed logarithm by

$$(42) \quad \ln_\phi(u) = \int_1^u dv \frac{1}{\phi(v)}, \quad u > 0.$$

It satisfies  $\ln_\phi(1) = 0$  and

$$(43) \quad \frac{d}{du} \ln_\phi(u) = \frac{1}{\phi(u)}.$$

The natural logarithm is obtained with  $\phi(u) = u$ , The Tsallis  $q$ -logarithm is obtained with  $\phi(u) = u^q$  for  $q > 0$ .

**3.2. The  $\phi$ -exponential function.** The inverse of the function  $\ln_\phi(x)$  is called the  $\phi$ -exponential and is denoted  $\exp_\phi(x)$ . It can be written in terms of a function  $\psi$  on  $\mathbb{R}$  defined by:

$$(44) \quad \psi(u) = \begin{cases} \phi(\exp_\phi(u)), & \text{if } u \text{ is in the range of } \ln_\phi, \\ 0, & \text{if } u \text{ is too small,} \\ +\infty, & \text{if } u \text{ is too large.} \end{cases}$$

Clearly is  $\phi(u) = \psi(\ln_\phi(u))$  for all  $u > 0$ . Then  $\exp_\phi$  is defined by:

$$(45) \quad \exp_\phi(u) = 1 + \int_0^u dv \psi(v).$$

It is clear that  $\exp_\phi(0) = 1$  and

$$(46) \quad \frac{d}{du} \exp_\phi(u) = \psi(u).$$

**3.3. Deduced Logarithms.** The deduced logarithm is defined by

$$(47) \quad \omega_\phi(u) = u \int_0^{1/u} dv \frac{v}{\phi(v)} - \int_0^1 dv \frac{v}{\phi(v)} - \ln_\phi \frac{1}{u}.$$

It satisfies  $\omega_\phi(1) = 0$  and that

$$(48) \quad \frac{d}{du} \omega_\phi(u) = \int_0^{1/u} dv \frac{v}{\phi(v)}.$$

Introduce a function:

$$(49) \quad \chi(u) = \left[ \int_0^{1/u} dv \frac{v}{\phi(v)} \right]^{-1},$$

so one can see that the deduced logarithmic function is the  $\chi$ -logarithm function:

$$(50) \quad \omega_\phi(u) = \ln_\chi(u).$$



**3.4. The  $\phi$ -entropy.** The  $\phi$ -entropy is defined by [6]:

$$(51) \quad H_\phi(p) = \sum_{i=1}^n p_i \ln_\chi(1/p_i),$$

After a short calculation:

$$(52) \quad H_\phi(p) = - \sum_{i=1}^n p_i \int_1^{p_i} \frac{1}{v^2} \left[ \int_0^v du \frac{u}{\phi(u)} \right] dv.$$

For our purpose, we will define

$$(53) \quad \tilde{H}_\phi(p) = \sum_{i=1}^n p_i \int_{p_i}^{+\infty} \frac{1}{v^2} \left[ \int_0^v du \frac{u}{\phi(u)} \right] dv$$

in order to remove some irrelevant constants. We will call this the *modified  $\phi$ -entropy*.

**3.5. The entropy function  $H_{BE}$  and  $H_{FD}$  as modified  $\phi$ -entropy.**

Define the following family of functions parameterized by  $\epsilon$ :

$$(54) \quad \phi_\epsilon(p) = p(1 + \epsilon p).$$

We have

$$\begin{aligned} \tilde{H}_{\phi_\epsilon}(p) &= \sum_{i=1}^n p_i \int_{p_i}^{\infty} \frac{1}{v^2} \left[ \int_0^v du \frac{u}{u(1 + \epsilon u)} \right] dv \\ &= \sum_{i=1}^n p_i \int_{p_i}^{\infty} \frac{1}{\epsilon v^2} \ln |1 + \epsilon v| dv \\ &= \sum_{i=1}^n \left( \frac{1 + \epsilon p_i}{\epsilon} \ln(1 + \epsilon p_i) - p_i \ln p_i \right) \\ &= H_\epsilon. \end{aligned}$$

In particular, the entropy functions  $H_{BE}$ ,  $H_{BGS} + 1$  and  $H_{FD}$  are the modified  $\phi_\epsilon$ -entropy functions for  $\epsilon = +1$ ,  $0$  and  $-1$  respectively.

**3.6. Bose-Einstein weight function and Fermi-Dirac weight function as modified  $\phi$ -exponential function.** Similarly, we defined the modified  $\phi$ -logarithm function by:

$$(55) \quad \tilde{\ln}_\phi(u) = - \int_u^\infty dv \frac{1}{\phi(v)}, \quad u > 0,$$

and define the modified  $\phi$ -exponential function  $\widetilde{\exp}_\phi$  as its inverse function.

For the function  $\phi_\epsilon(p) = p(1 + \epsilon p)$ , we have

$$(56) \quad \widetilde{\ln}_{\phi_\epsilon}(u) = - \int_u^\infty dv \frac{1}{v(1 + \epsilon v)} = \ln |1 + \epsilon u| - \ln(u).$$

It follows that

$$(57) \quad u = \widetilde{\exp}_{\phi_\epsilon}(\eta) = \frac{1}{e^\eta - \epsilon},$$

and so we have

$$(58) \quad p_\epsilon(E) = \widetilde{\exp}_{\phi_\epsilon}(a + bE).$$

#### 4. FRACTIONAL EXCLUSION STATISTICS

In this section, we treat the case of fractional exclusion statistics of Haldane [3]. We refer to [5, Chapter 5] for backgrounds. Since the ideas are similar, we will be very brief.

Wu [8] has derived the following formula for the weight function:

$$(59) \quad p(g) = \frac{1}{\omega(\eta) + g},$$

where the function  $\omega(\eta)$  satisfies the functional equation:

$$(60) \quad \omega(\eta)^g (1 + \omega(\eta))^{1-g} = e^\eta.$$

For the special cases of  $g = 0$  and  $1$  we have  $w(\eta) = e^{-\eta} - 1$  and  $w(\eta) = e^{-\eta}$ , and so we recover the Bose-Einstein and the Fermi-Dirac statistics respectively for  $\eta = -(a + bE)$ . This weight function can be derived by maximizing the following family of entropy functions parameterized by  $g$ :

$$(61) \quad H_g(p) = (1 + (1 - g)p) \ln(1 + (1 - g)p) - (1 - gp) \ln(1 - gp) - p \ln p,$$

under the constraints (2) and (5). This is because

$$(62) \quad \frac{\partial H_g}{\partial p} = \ln \frac{(1 + (1 - g)p)^{1-g} (1 - gp)^g}{p},$$

and so by the method of Lagrange multiplier one can get:

$$(63) \quad \frac{(1 + (1 - g)p)^{1-g} (1 - gp)^g}{p} = e^{-(a+bE)}.$$

One can readily check that

$$(64) \quad H_g = \tilde{H}_{\phi_g}(p),$$

$$(65) \quad p_g(E) = \widetilde{\exp}_{\phi_g}(a + bE),$$

for the following function:

$$(66) \quad \phi_g(p) = p(1 - gp)(1 + (1 - g)p).$$

## 5. CONCLUSIONS AND PROSPECTS

In this paper we have generalized Jaynes' derivation of Boltzmann-Gibbs statistics by the Principle of Maximum Entropy. A family  $H_\epsilon$  of entropy functions has been introduced to give a unified derivation of Bose-Einstein, Boltzmann-Gibbs and Fermi-Dirac statistics together with the interpolating Acharya-Swamy statistics. The family  $H_\epsilon$  turns out to be a special case of Naudts'  $\phi$ -entropy and the probabilities are  $\phi$ -exponentials, with suitable modifications, for  $\phi$  given by  $\phi_\epsilon(p) = p + \epsilon p^2$ . A different interpolation of Bose-Einstein and Fermi-Dirac statistics is given by the  $\phi_g$ -exponential function and the corresponding entropy function is given by the  $\phi_g$ -logarithm function, for  $\phi_g(p) = p(1 - gp)(1 + (1 - g)p)$ . The two series of functions  $\phi_\epsilon$  and  $\phi_g$  suggest us to study more general deformation of  $\phi = p$  given by  $\phi_{\mathbf{T}}(p) = p - \sum_{n \geq 2} T_{n-1} p^n$ . In a subsequent work we will verify that other statistics interpolating Bose-Einstein statistics and Fermi-Dirac statistics are  $\phi_{\mathbf{T}}$ -exponential functions and are critical point of  $\phi_{\mathbf{T}}$ -entropy functions. Furthermore, any deformation of the Boltzmann-Gibbs-Shannon entropy in some suitable sense can be obtained as a  $\phi_{\mathbf{T}}$ -entropy. We will use such considerations to establish a connection with string theory. More precisely, we will show that some computations in string theory can be used to generate interpolating statistics.

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